Gaussian phase-space representations for fermions

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We introduce a positive phase-space representation for fermions, using the most general possible multi-mode Gaussian operator basis. The representation generalizes previous bosonic quantum phase-space methods to Fermi systems. We derive equivalences between quantum and stochastic moments, as well as operator correspondences that map quantum operator evolution onto stochastic processes in phase space. The representation thus enables first-principles quantum dynamical or equilibrium calculations in many-body Fermi systems. Potential applications are to strongly interacting and correlated Fermi gases, including coherent behaviour in open systems and nanostructures described by master equations. Examples of an ideal gas and the Hubbard model are given, as well as a generic open system, in order to illustrate these ideas.

I. INTRODUCTION

The study of strongly correlated Fermi gases is one of the most active areas in modern condensed matter and AMO physics. In quantum degenerate electron gases, improvements in condensed matter materials have led to sophisticated experiments, typically in reduced dimensional environments. Many interesting quantum phenomena are observed in these systems, including such features as the quantum Hall effect[1], metal-insulator phase-transitions[2], high T-c superconductors[3], and single electron gates in nanostructures[4].

Recently, pioneering experiments in strongly-interacting ultra-cold Fermi gases have opened up novel experiments of unprecedented simplicity and precision, both in the BEC-BCS cross-over regime[5], and in lattices[6]. The underlying atomic interactions are extremely well-understood, and the dynamics, interactions and geometry are all highly adaptable. Measurement techniques are also rapidly improving, with direct measurements of collective modes[7], thermodynamic properties[8], vortices[9], and even momentum correlations being recently reported[10].

This situation provides a substantial opportunity to develop and test first-principles theoretical methods for the investigation of correlations and dynamical effects in quantum degenerate Fermi gases. To this end, we introduce a generalised phase-space representation for correlated fermionic systems. The representation is based on a Gaussian operator basis for fermionic density operators. Like the analogous basis for bosons[11], the fermionic operator basis enables the representation of arbitrary physical density operators as a positive distribution over a phase space. This representation allows quantum evolution, either in real time or in inverse temperature, to be viewed as a stochastic evolution of covariances or Green's functions.

Phase-space methods based on coherent states[12] have long been used for bosonic systems, with great success. These approaches include the Wigner function[13], the Q-function[14], as well as the well-known Glauber-Sudarshan P-function[15], and its generalizations[16,17]. The early methods based on classical phase spaces were later generalized to give the positive-P distribution[18], which has proved a successful way to simulate quantum many-body systems from first principles[19]. This method reduces quantum dynamics to the time evolution of a positive distribution on an over-complete basis set of coherent state projection operators, which are special cases of the bosonic Gaussian operators. Applications have been to quantum statistics of lasers[20], superfluorescence[21], parametric amplifiers[18,22], quantum solitons[23], as well as quantum dynamics[24] and thermal correlations[25] in Bose-Einstein condensates.

Fermionic phase-space representations are relevant to a long-standing problem in theoretical physics, which is the sign problem that occurs in many-body fermionic wave-functions[26,27,28]. There are many different approximate techniques that can be used, but the intention of this paper is to establish fundamentally exact procedures to treat the Fermi sign problem. As shown in[29], the Gaussian method can be applied to the difficult case of the repulsive Hubbard model[30]. Here we concentrate on the foundational issues of the Gaussian representation method, presenting the general identities required to apply the method to a wide range of problems in fermionic many-body physics, including both ultra-cold atomic and condensed matter systems.

To proceed, we make use of three important results, proved elsewhere[31]:

- the Gaussian fermion operators form a complete basis for any physical density operator,
- the distribution can always be chosen positive, and
- there are mappings to a second-order differential form for all two-body operators.

From these properties, we show that positive-definite Fokker-Planck equations exist for many-body fermionic systems, provided that the distribution tails remain sufficiently bounded. Such Fokker-Planck equations enable first-principles stochastic simulation methods, either in real time or at finite temperature. As is usual in such

methods, care must be taken with sampling errors and boundary terms due to the distribution tails. Due to the non-uniqueness of the representation, there is a type of gauge freedom in the choice of stochastic equation. We show how this stochastic gauge freedom, which has been successfully used to remove boundary terms in bosonic representations[32], can in principle also be used here.

Representations for fermionic density operators were introduced by Cahill and Glauber[33] using fermionic coherent states[34]. These provide a means of defining quasi-probabilities for fermionic states analogous to the well-known bosonic distributions[33,35]. However, the resulting quasi-probabilities are functions of non-commuting Grassmann variables, and are thus not directly computationally accessible. Nevertheless, fermion coherent states and Grassmann algebra are useful for deriving analytical results in Fermi systems.

The Gaussian method introduced here overcomes the problems inherent in using Grassmann algebra variables. The Gaussian expansion utilises an operator basis constructed from pairs of operators, instead of a state-vector basis. Because pairs of fermion operators obey commutation relations rather than anti-commutation relations, a natural solution of the anticommutation problem is achieved. The resulting phase space thus exists on a domain of commuting c-numbers, rather than anti-commuting Grassmann variables. Furthermore, the phase-space equations obviate the need to evaluate large determinants in simulations. This method substantially generalizes and extends earlier phase-space techniques used in quantum optics to treat electronic transitions in atoms[20,36]. It is different to auxiliary field quantum Monte Carlo methods[37] in condensed matter theory, which use Gaussian operators, but involve path integrals rather than positive expansions of the density matrix.

We begin in Sec.II by defining the Gaussian operator basis on which the representation is based, and introducing some convenient notations. In Sec.III, we define the Gaussian representation as an expansion in Gaussian operators, and then show how the representation establishes a novel class of exact Monte-Carlo type methods for simulating the real-time dynamics or finite-temperature equilibrium of a quantum system. We show how to map quantum operator evolution onto a set of stochastic (real or complex) differential equations, and give the correspondences necessary to calculate physical moments.

Finally, in Sec. V, we give examples of the application of the method. These are intended to be illustrative rather than exhaustive, and further examples and applications in greater detail will be given elsewhere. In particular, we note that any nonlinear application requires a careful analysis of the issues of sampling error and boundary term behaviour. For simplicity, we focus on the ideal Fermi gas, a generic open system master equation and the finite temperature Hubbard model, as well as showing how to apply gauges to modify the drift evolution.

II. GAUSSIAN OPERATORS

Before discussing the Gaussian representation, we first introduce the fermion operators on which it is based. Fermionic Gaussian operators are defined as exponentials of quadratic forms in the Fermi annihilation or creation operators. This simple definition encompasses a wide range of physical applicability. Obviously, it includes the well-known thermal density matrices of the free field. Since the definition includes quadratic forms involving pairs of annihilation or creation operators, it also encompasses the pure-state density matrices that correspond to the BCS states used in superconductivity.

A more subtle issue is that the definition is not restricted to Hermitian operators. This has the advantage of leading to completeness properties that are much stronger than if the definition were restricted to only Hermitian operators. Some of these issues are discussed elsewhere, in a more formal derivation of the mathematical properties of the Gaussian operators[31].

A. Notation

Before giving mathematical results, we summarize the notation that will be used. We can decompose a given fermionic system into a set of M orthogonal single-particle modes, or orbitals. With each of these modes, we associate creation and annihilation operators $\widehat{b}_j^\dagger$ and $\widehat{b}_j$, with anticommutation relations

$$\begin{aligned}\left[\widehat{b}_k,\widehat{b}_j^\dagger\right]_+ &= \delta_{kj}\\ \left[\widehat{b}_k,\widehat{b}_j\right]_+ &= 0\ ,\end{aligned} \tag{2.1}$$

where $j,k = 1...M$. Thus, $\widehat{\boldsymbol{b}}$ is a column vector of the M annihilation operators, and $\widehat{\boldsymbol{b}}^\dagger$ is a row vector of the corresponding creation operators.

For products of operators, we make use of normal and antinormal ordering concepts. Normal ordering, denoted by $:\cdots:$, is defined as in the bosonic case, with all annihilation operators to the right of the creation operators, except that each pairwise reordering involved induces a sign change, e. g. $:\widehat{b}_i\widehat{b}_j^\dagger: = -\widehat{b}_j^\dagger\widehat{b}_i$. The sign changes are necessary so that the anticommuting natures of the Fermi operators can be accommodated without ambiguity.

To enable the general Gaussian operator to be written in a compact form, we use an extended-vector notation:

$$\underline{\widehat{b}} = \begin{pmatrix}\widehat{\boldsymbol{b}}\\ \widehat{\boldsymbol{b}}^{\dagger T}\end{pmatrix}\ , \tag{2.2}$$

is defined as an extended column vector of all $2M$ operators, with an adjoint row vector defined as

$$\underline{\widehat{b}}^\dagger = (\widehat{\boldsymbol{b}}^\dagger, \widehat{\boldsymbol{b}}^T)\ . \tag{2.3}$$

Throughout the paper, we print vectors of length M and $M \times M$ matrices in bold type, and index them where necessary with Latin indices: $j = 1, ..., M$. Vectors of length $2M$ we denote with an underline, while $2M \times 2M$ matrices are indicated by a double underline. These extended vectors and matrices are indexed where necessary with Greek indices: $\mu = 1, ..., 2M$. For further examples of this notation, see[11,31]. More general kinds of vectors are denoted with an arrow notation: $\overrightarrow{\lambda}$.

B. Definition of the Gaussian operator

We define a Gaussian operator to be any normally ordered, Gaussian form of annihilation and creation operators. Like a complex number Gaussian, the operator Gaussian is an exponential of a quadratic form, with the exponential defined by its series representation. The most general Gaussian form is a cumbersome object to manipulate, unless products of odd numbers of operators are excluded. Fortunately, restricting the set of Gaussians to those containing only even products can be physically justified on the basis of superselection rules for fermions. Because it is constructed from pairs of operators, this type of Gaussian operator contains no Grassmann variables.

With the extended-vector notation, we can write any general Gaussian operator $\widehat{\Lambda}$ as:

$$\widehat{\Lambda}(\overrightarrow{\lambda}) = \Omega \frac{1}{\mathcal{N}} : \exp\left[-\underline{\widehat{b}}^{\dagger} \underline{\underline{\Sigma}} \underline{\widehat{b}}/2\right] : , \tag{2.4}$$

where Ω is an amplitude, $\mathcal{N}$ is a normalizing factor defined so that $\mathrm{Tr}\left[\widehat{\Lambda}(\overrightarrow{\lambda})\right] = \Omega$, and $\underline{\underline{\Sigma}}$ is a $2M \times 2M$ complex matrix. For later identification with physical observables, it proves useful to write $\underline{\underline{\Sigma}}$ in the form:

$$\underline{\underline{\Sigma}} = \left(\underline{\underline{\sigma}}^{-1} - 2\underline{\underline{I}}\right), \tag{2.5}$$

where $\underline{\underline{\sigma}}$ is a generalised covariance matrix and $\underline{\underline{I}}$ is the constant matrix is defined as

$$\underline{\underline{I}} = \begin{bmatrix} -\mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{bmatrix}, \tag{2.6}$$

It is convenient to introduce complex $M \times M$ matrices $\mathbf{n}$ and $\tilde{\mathbf{n}} = \mathbf{I} - \mathbf{n}$ which, as we show later, correspond to normal Green's function for particles and holes respectively, and two independent antisymmetric complex $M \times M$ matrices $\mathbf{m}$ and $\mathbf{m}^{+}$ that correspond to anomalous Green's functions. These are related to the covariance matrix $\underline{\underline{\sigma}}$ by

$$\begin{bmatrix} -\tilde{\mathbf{n}}^{T} & \mathbf{m} \\ \mathbf{m}^{+} & \tilde{\mathbf{n}} \end{bmatrix} = \begin{bmatrix} \mathbf{n^{T}} - \mathbf{I} & \mathbf{m} \\ \mathbf{m}^{+} & \mathbf{I} - \mathbf{n} \end{bmatrix} = \frac{1}{2}\left(\underline{\underline{\sigma}} - \underline{\underline{\sigma}}^{+}\right), \tag{2.7}$$

where '+' denotes a generalised transpose operation defined by

$$\begin{bmatrix} \mathbf{a} & \mathbf{b} \\ \mathbf{c} & \mathbf{d} \end{bmatrix}^{+} \equiv \begin{bmatrix} \mathbf{d} & \mathbf{c} \\ \mathbf{b} & \mathbf{a} \end{bmatrix}^{T} . \tag{2.8}$$

Any Gaussian operator can always be written with a covariance matrix that has the antisymmetry $\underline{\underline{\sigma}} = -\underline{\underline{\sigma}}^{+}$.

The Gaussian operators are defined here in terms of the full $1 + p = 1 + 4M^2$ amplitude plus covariance matrix components. Alternatively, we can include just the parameters $\overrightarrow{\lambda}$ that lead to distinguishable Gaussians, where

$$\overrightarrow{\lambda} = (\Omega, \mathbf{n}, \mathbf{m}, \mathbf{m}^{+}) , \tag{2.9}$$

giving only $1 + p = 1 + M(2M - 1)$ parameters. We will index over the phase-space variables with the notation λ_a, $a = 0, \ldots p$. For simplicity, we generally deal with the full, unconstrained $\underline{\underline{\sigma}}$ matrices.

The normalisation $\mathcal{N}$ contains a Pfaffian whose square is equal to the determinant of the matrix. We will show that $\mathcal{N}$ does not appear explicitly in later results. The additional variable Ω plays the role of a weighting factor in the expansion. This allows us to represent unnormalised density operators like $\exp(-\beta\widehat{H})$, and to introduce stochastic gauges that change these relative weighting factors in order to stabilize trajectories.

C. Moments

Just as with classical Gaussian forms, these generalised fermionic Gaussians are completely characterised by their first order moments (to within a weight factor):

$$\begin{aligned} \mathrm{Tr}\left[\widehat{b}_i \widehat{b}_j \widehat{\Lambda}\right] &= \Omega m_{ij}, \\ \mathrm{Tr}\left[\widehat{b}_i^{\dagger} \widehat{b}_j \widehat{\Lambda}\right] &= \Omega n_{ij} , \\ \mathrm{Tr}\left[\widehat{b}_j \widehat{b}_i^{\dagger} \widehat{\Lambda}\right] &= \Omega \tilde{n}_{ij} , \\ \mathrm{Tr}\left[\widehat{b}_i^{\dagger} \widehat{b}_j^{\dagger} \widehat{\Lambda}\right] &= \Omega m_{ij}^{+} . \end{aligned} \tag{2.10}$$

If the Gaussian operator happens to be a physical density matrix, these quantities correspond to the first-order correlations or Green's functions. Thus, in many-body terminology, $\mathbf{n}$ and $\tilde{\mathbf{n}}$ are the normal Green's functions of particles and holes, respectively, and $\mathbf{m}$ and $\mathbf{m}^{+}$ are anomalous Green's functions. From this we see that, for the subset of Gaussians that are physical density matrices, we must have that $\mathbf{m}^{\dagger}$=$\mathbf{m}^{+}$, and $\mathbf{n}^{\dagger}$=$\mathbf{n}$. Furthermore, $\mathbf{n}$ and $\tilde{\mathbf{n}}$ must be positive semi-definite (because $0 \leq \langle \widehat{n}_{jj} \rangle \leq 1$) .

More generally, the phase-space function $O(\overrightarrow{\lambda})$ corresponding to the normally ordered operator $\widehat{O}$ is defined as a phase-space correspondence, according to:

$$O(\overrightarrow{\lambda}) \equiv \left\langle \widehat{O} \right\rangle_{\overrightarrow{\lambda}} \equiv \mathrm{Tr}\left(\widehat{O}\,\widehat{\Lambda}(\overrightarrow{\lambda})\right)/\Omega . \tag{2.11}$$

For higher-order moments, a form of Wick's theorem applies to any normally ordered product. One simply writes down the sum of all distinct factorisations into pairs, with a minus sign in front of any product that is an odd permutation of the original form. The term distinct factorization means that neither permutation of pair ordering nor re-ordering inside a pair is regarded as significant, since these do not change the result. Thus an N-th order correlation (expectation value of a product of $2N$ operators), is the sum of $2N!/(2^N N!)$ distinct terms, as follows,

$$\left\langle :\widehat{b}_{\mu_1}....\widehat{b}_{\mu_{2N}}: \right\rangle_{\overrightarrow{\lambda}} = \sum_P (-1)^P \left\langle :\widehat{b}_{\mu_{P(1)}}\widehat{b}_{\mu_{P(2)}}: \right\rangle_{\overrightarrow{\lambda}} \times ... \times \left\langle :\widehat{b}_{\mu_{P(2N-1)}}\widehat{b}_{\mu_{P(2N)}}: \right\rangle_{\overrightarrow{\lambda}} . \quad (2.12)$$

Here the sum is over all $2N!/(2^N N!)$ distinct pair permutations $P(1), ..., P(2N)$ of $1, ..., 2N$, and where $(-1)^P$ is the parity of the permutation (i.e. the number of pair-wise transpositions required to perform the permutation).

Thus, for example, the second-order number correlation moment is:

$$\left\langle \widehat{b}_i^\dagger \widehat{b}_j^\dagger \widehat{b}_j \widehat{b}_i \right\rangle_{\overrightarrow{\lambda}} = n_{ii}n_{jj} - n_{ij}n_{ji} + m_{ij}^+ m_{ji} . \quad (2.13)$$

D. Generalised thermal states

An important subset of the Gaussian operators is the set of generalized thermal operators, for which $\mathbf{m} = \mathbf{m}^+ = \mathbf{0}$. These include the canonical density matrices for free Fermi gases in the case that $\mathbf{n}$, and $\tilde{\mathbf{n}}$ are each Hermitian and positive definite. More generally, however, we do not require $\mathbf{n}$ to be Hermitian. In all cases, the generalized thermal operators in normally ordered Gaussian form can be written most directly in terms of the hole population, $\tilde{\mathbf{n}} = \mathbf{I} - \mathbf{n}$:

$$\widehat{\Lambda}(\overrightarrow{\lambda}) = \Omega \det[\tilde{\mathbf{n}}] : \exp\left[\widehat{\mathbf{b}}^\dagger \left(\tilde{\mathbf{n}}^{-1} - 2\mathbf{I}\right)^T \widehat{\mathbf{b}}\right] : . \quad (2.14)$$

Of course, there is a symmetry here: in an antinormally ordered Gaussian, the role of $\widehat{\mathbf{b}}^\dagger$ and $\widehat{\mathbf{b}}$ is reversed, and consequently so is the role of $\mathbf{n}$ and $\tilde{\mathbf{n}}$. Our choice of normal ordering is in fact arbitrary from a physical point of view, and antinormal ordering would also serve our purpose equally well, provided all the identities were redefined.

By comparison, the usual canonical form of the fermionic thermal state with a diagonal Hamiltonian $H = \widehat{\mathbf{b}}^\dagger \omega \widehat{\mathbf{b}}$ and a chemical potential μ, is an unordered form, namely:

$$\widehat{\rho}(\tau) = \exp\left[\tau \widehat{\mathbf{b}}^\dagger (\mu - \omega) \widehat{\mathbf{b}}\right] / Z . \quad (2.15)$$

Here Z is the partition function and $\tau = 1/k_B T$ is the inverse temperature. In this case, the mean occupation numbers are diagonal, and are well-known. They are given by the Fermi-Dirac distribution;

$$\left\langle \widehat{b}_i^\dagger \widehat{b}_j \right\rangle = \bar{n}_{ij} = \frac{\delta_{ij}}{1 + e^{\tau(\omega_i - \mu)}} . \quad (2.16)$$

However, both Gaussian forms are equivalent. A normally ordered thermal Gaussian can always be chosen so that $\mathbf{n}$ is Hermitian, and hence $\widehat{\rho}(\tau) = \widehat{\Lambda}(\overrightarrow{\lambda})$ if and only if $\Omega = 1$ and $n_{ij} = \bar{n}_{ij}$.

A rather trivial example is the vacuum state, in which $\mathbf{n} = \mathbf{0}$, so that:

$$\widehat{\Lambda}(1, \mathbf{0}, \mathbf{0}, \mathbf{0}) = |\mathbf{0}\rangle\langle\mathbf{0}| = : \exp\left[-\widehat{\mathbf{b}}^\dagger \widehat{\mathbf{b}}\right] : . \quad (2.17)$$

We emphasize that since the Gaussian forms used here are not necessarily Hermitian, the generalized thermal operators are a much larger set of operators than the usual canonical thermal density matrices.

E. Generalised BCS states

A second important subset of the Gaussian operators is the generalisation of the Bardeen-Cooper-Schreiffer (BCS) states, which are an excellent approximation to the ground state of a weakly interacting (BCS) superconductor. The BCS states are the fermionic equivalent of the squeezed states found in quantum optics, and are composed only of correlated fermion pairs. In the case of fermions, these are the fundamental pure states that carry phase information. In Bose gases, coherent states can also carry phase information (as in a laser or Bose-Einstein condensate), but the fermionic equivalent of these is an unphysical Grassmann coherent state.

An unnormalized pure BCS state is defined as[38]:

$$|\Psi_{\rm BCS}\rangle = \exp\left[\widehat{\mathbf{b}}^\dagger \mathbf{g} \widehat{\mathbf{b}}^\dagger / 2\right] |\mathbf{0}\rangle , \quad (2.18)$$

so that the corresponding density matrix is:

$$\begin{aligned} \widehat{\rho}_{\rm BCS} &= |\Psi_{\rm BCS}\rangle\langle\Psi_{\rm BCS}| \\ &= \exp\left[\widehat{\mathbf{b}}^\dagger \mathbf{g} \widehat{\mathbf{b}}^\dagger / 2\right] |\mathbf{0}\rangle\langle\mathbf{0}| \exp\left[\widehat{\mathbf{b}} \mathbf{g}^\dagger \widehat{\mathbf{b}} / 2\right] \\ &= : \exp\left[\widehat{\mathbf{b}}^\dagger \mathbf{g} \widehat{\mathbf{b}}^\dagger / 2 - \widehat{\mathbf{b}}^\dagger \widehat{\mathbf{b}} + \widehat{\mathbf{b}} \mathbf{g}^\dagger \widehat{\mathbf{b}} / 2\right] : . \end{aligned} \quad (2.19)$$

Apart from being unnormalized, this corresponds directly to a Gaussian in our normal form.

More general non-Hermitian BCS-type states are obtained on replacing $\mathbf{g}^\dagger$ by an independent matrix $\mathbf{g}^+$. This generalized BCS Gaussian has an extended covariance matrix of:

$$\underline{\underline{\sigma}} = \begin{bmatrix} (\mathbf{I} + \mathbf{g}\mathbf{g}^+)^{-1} & 0 \\ 0 & (\mathbf{I} + \mathbf{g}^+\mathbf{g})^{-1} \end{bmatrix} \begin{bmatrix} -\mathbf{I} & \mathbf{g} \\ \mathbf{g}^+ & \mathbf{I} \end{bmatrix} \quad (2.20)$$

Clearly, from this we can see that the occupation numbers and correlations for a generalized BCS state are given by:

$$\begin{aligned}\mathbf{n} &= \mathbf{g}^{+}\left(\mathbf{I}+\mathbf{g}\mathbf{g}^{+}\right)^{-1}\mathbf{g},\\ \tilde{\mathbf{n}} &= \left(\mathbf{I}+\mathbf{g}^{+}\mathbf{g}\right)^{-1}\\ \mathbf{m} &= \left(\mathbf{I}+\mathbf{g}\mathbf{g}^{+}\right)^{-1}\mathbf{g}\\ \mathbf{m}^{+} &= \mathbf{g}^{+}\left(\mathbf{I}+\mathbf{g}\mathbf{g}^{+}\right)^{-1},\end{aligned} \tag{2.21}$$

which gives the expected result that $\mathbf{m}^{+}\mathbf{m}=\tilde{\mathbf{n}}\mathbf{n}$.

In summary, the usual BCS states have a density matrix which is Gaussian, and has $\mathbf{g}^{+}=\mathbf{g}^{\dagger}$. These pure states exist as a subset of a more general class of BCS-like Gaussian operators. This class also includes operators which have $\mathbf{g}^{+}\neq\mathbf{g}^{\dagger}$, and are therefore not Hermitian. While these operators do not correspond to any physical state, a linear combination of them - provided the result is Hermitian and positive-definite - can still correspond to a possible physical fermionic many-body state.

III. GAUSSIAN REPRESENTATION

While the Gaussian operators include a large and interesting set of physical density operators, there are many cases where the existence of interparticle interactions leads to more general fermionic states whose correlations are of more complex, non-Gaussian forms. In all such cases, the overall physical density operator can still be expressed as a positive distribution over the Gaussian operators. Furthermore, any two-body operator acting on a generalised Gaussian can be written as a second-order derivative. These important results, proved in[31], means that probabilistic, random sampling methods may be used to calculate physical observables, as we show below.

A. Definition

The Gaussian representation for fermion operators is defined as an expansion of the density matrix for any physical state $\widehat{\rho}(t)$ as a distribution over the Gaussian basis. That is:

$$\widehat{\rho}(t)=\int P(\overrightarrow{\lambda},t)\widehat{\Lambda}(\overrightarrow{\lambda})d\overrightarrow{\lambda}\ , \tag{3.1}$$

where the expansion coefficients are normalised to one:

$$\int P(\overrightarrow{\lambda},t)d\overrightarrow{\lambda}=1\ . \tag{3.2}$$

This expansion defines a type of phase-space representation of the state: the vector $\overrightarrow{\lambda}$ of Gaussian parameters becomes a generalised phase-space coordinate, the function $P(\overrightarrow{\lambda},t)$ is then a probability distribution function over the generalised phase space, and $d\overrightarrow{\lambda}=d^{2(p+1)}\overrightarrow{\lambda}$ is the phase-space integration measure.

B. Moments

Some basic properties of $P(\overrightarrow{\lambda},t)$ follow from those of the Gaussian operators. For example, using the normalisation of the Gaussian operators we find that

$$\mathrm{Tr}\left[\widehat{\rho}\right]\ =\ \int P(\overrightarrow{\lambda},t)\Omega d\overrightarrow{\lambda}\equiv\overline{\Omega}. \tag{3.3}$$

Thus the normalised distribution P can represent unnormalised density operators by incorporating the normalisation into the mean weight $\overline{\Omega}$.

More generally, the expectation value of an operator $\widehat{O}$ evaluates to

$$\begin{aligned}\left\langle\widehat{O}\right\rangle &\equiv \mathrm{Tr}\left[\widehat{O}\,\widehat{\rho}\right]/\mathrm{Tr}\left[\widehat{\rho}\right]\\ &= \int P(\overrightarrow{\lambda},t)\mathrm{Tr}\left[\widehat{O}\,\widehat{\Lambda}\right]d\overrightarrow{\lambda}/\overline{\Omega}\\ &\equiv \left\langle O(\overrightarrow{\lambda})\right\rangle_{P}\ ,\end{aligned} \tag{3.4}$$

where the weighted average $\langle\ldots\rangle_{P}$ is defined as:

$$\left\langle O(\overrightarrow{\lambda})\right\rangle_{P}=\int P(\overrightarrow{\lambda},t)\Omega O(\overrightarrow{\lambda})d\overrightarrow{\lambda}/\overline{\Omega}\ . \tag{3.5}$$

The phase-space function $O(\overrightarrow{\lambda})$ corresponding to the operator $\widehat{O}$ is defined as previously, using the generalised Wick result of Eq. (2.12).

Physical quantities thus correspond to (weighted) moments of P. For example, from traces evaluated in Sec. II C, we find that the normal and anomalous Green's functions correspond to first order moments:

$$\begin{aligned}\left\langle\widehat{b}_{i}\widehat{b}_{j}\right\rangle &= \langle m_{ij}\rangle_{P}\ ,\\ \left\langle\widehat{b}_{i}^{\dagger}\widehat{b}_{j}\right\rangle &= \langle n_{ij}\rangle_{P}\ ,\\ \left\langle\widehat{b}_{i}^{\dagger}\widehat{b}_{j}^{\dagger}\right\rangle &= \langle m_{ij}^{+}\rangle_{P}\ .\end{aligned} \tag{3.6}$$

Number-number correlations correspond to averages of products of these moments:

$$\langle:\widehat{n}_{i}\widehat{n}_{j}:\rangle\ =\ \left\langle n_{ii}n_{jj}-n_{ij}n_{ji}+m_{ij}^{+}m_{ji}\right\rangle_{P}\ , \tag{3.7}$$

where $\widehat{n}_{i}\equiv\widehat{b}_{i}^{\dagger}\widehat{b}_{i}$.

Similarly, higher-order correlations correspond to higher-order moments, the form of which are also determined by the generalised Wick result of Eq. (2.12).

We note that the expectation value of any odd product of operators must vanish e.g. $\left\langle\widehat{b}_{i}\right\rangle=0$. Thus the distribution cannot represent a superposition of states whose total number differ by an odd number. Such superposition states we exclude from our definition of physical state, as they are not generated by evolution under any known physical Hamiltonian. The Gaussian distribution can, however, represent systems in which particles are

coherently added or removed in pairs, leading to nonzero anomalous correlations $\langle m_{ij}\rangle_P$. On the other hand, if the total number of particles is conserved or changed only via contact with a thermal reservoir, then the anomalous correlations will be identically zero and we can represent the system via an expansion in only the thermal subset of Gaussian operators.

IV. TIME EVOLUTION

Here we show how these positive representations of density matrices can be put to use. By use of these representations, any quantum evolution arising from one and two-body interactions can be sampled by classical stochastic processes. To see this, note that the time evolution of a density operator is determined by a master equation, of the general form

$$\frac{d}{dt}\widehat{\rho}(t) \;=\; \widehat{L}\,[\widehat{\rho}(t)]\,, \tag{4.1}$$

where the $\widehat{L}$ is a superoperator that pre- and post-multiplies the density operator by combinations of annihilation and creation operators.

A. Types of evolution

We consider three general time-evolution categories:

Hamiltonian quantum dynamics

For unitary evolution in real time, the superoperator is a commutator with the Hamiltonian:

$$\widehat{L}\,[\widehat{\rho}] \;=\; -\frac{i}{\hbar}\left[\widehat{H},\widehat{\rho}\right]\,. \tag{4.2}$$

Irreversible quantum dynamics

More generally, for an open quantum system, there will be additional terms of Lindblad form[39,40] to describe the coupling to the environment:

$$\widehat{L}\,[\widehat{\rho}] \;=\; -\frac{i}{\hbar}\left[\widehat{H},\widehat{\rho}\right]+\sum_K\left(2\widehat{O}_K\widehat{\rho}\,\widehat{O}_K^\dagger-[\widehat{O}_K^\dagger\widehat{O}_K,\widehat{\rho}]_+\right), \tag{4.3}$$

where the operators $\widehat{O}_K$ depend on the correlations of the environment or reservoir, within the Markov approximation.

Thermal equilibrium ensemble

To calculate the canonical thermal equilibrium state at temperature $T=1/k_B\tau$, one can solve an inverse temperature equation for the unnormalised density operator:

$$\frac{d}{d\tau}\widehat{\rho} \;=\; -\frac{1}{2}[\widehat{H}-\mu\widehat{N}\,,\widehat{\rho}]_+\,, \tag{4.4}$$

the solution of which will generate the unnormalised density operator for a grand canonical distribution: $\rho(\tau)=\exp[-\tau(\widehat{H}-\mu\widehat{N})]$.

B. Operator Mappings

We wish to show how to transform a general operator time-evolution equation (Eq. (4.1)) into a Fokker-Planck equation for the distribution, and hence into a stochastic equation. A crucial part of this procedure is to be able to transform the operator equations into a differential form.

The first step is to substitute for $\widehat{\rho}$ the expansion in Eq. (3.1):

$$\int\frac{dP(\overrightarrow{\lambda},t)}{dt}\widehat{\Lambda}(\overrightarrow{\lambda})d\overrightarrow{\lambda} \;=\; \int P(\overrightarrow{\lambda},t)\,\widehat{L}\left[\widehat{\Lambda}(\overrightarrow{\lambda})\right]d\overrightarrow{\lambda}\,. \tag{4.5}$$

Second, we use the differential identities derived in[31] to convert the superoperator $\widehat{L}\left[\widehat{\Lambda}\right]$ into an operator $\mathcal{L}\left[\widehat{\Lambda}\right]$ that contains only derivatives of $\widehat{\Lambda}$. Next we integrate by parts to obtain, provided that no boundary terms arise,

$$\int\frac{dP(\overrightarrow{\lambda},t)}{dt}\widehat{\Lambda}(\overrightarrow{\lambda})d\overrightarrow{\lambda} \;=\; \int\mathcal{L}'\left[P(\overrightarrow{\lambda},t)\right]\widehat{\Lambda}(\overrightarrow{\lambda})d\overrightarrow{\lambda}\,, \tag{4.6}$$

where $\mathcal{L}'$ is a reordered form of $\mathcal{L}$, with a sign change to derivatives of odd order. Finally, we see that this equation holds if the distribution function satisfies the evolution equation

$$\frac{d}{dt}\;P(\overrightarrow{\lambda},t) = \;\mathcal{L}'\left[P(\overrightarrow{\lambda},t)\right]. \tag{4.7}$$

This procedure for going from the master equation for $\widehat{\rho}$ to the evolution equation for P can be implemented using a set of operator mappings, in which we introduce *anti*normal ordering as the opposite of normal ordering, and denote it via curly braces: $\{\widehat{b}_j^\dagger\widehat{b}_i\}=-\widehat{b}_i\widehat{b}_j^\dagger$. More generally, we can define nested orderings, in which the outer ordering does not reorder the inner one. For example, $\{:\widehat{\rho}\widehat{b}_j^\dagger:\widehat{b}_i\}=-\widehat{b}_i\widehat{b}_j^\dagger:\widehat{\rho}:$, where $\widehat{\rho}$ is some density operator. When ordering products that contain the density operator $\widehat{\rho}$, we do not change the ordering of $\widehat{\rho}$ itself; the other operators are merely reordered around it.

Including all possible orderings, we obtain the following mappings:

$$
\begin{aligned}
\widehat{\rho} &\longrightarrow -\frac{\partial}{\partial\Omega}\Omega P\,,\\
:\widehat{\rho}\,\underline{\widehat{b}}\,\underline{\widehat{b}}^{\dagger}: &\longrightarrow \left[\underline{\underline{\sigma}}^{(s)}+2\underline{\underline{\sigma}}\frac{\overleftrightarrow{\partial}}{\partial\underline{\underline{\sigma}}}\underline{\underline{\sigma}}\right]P\,,\\
:\left\{\widehat{\rho}\,\underline{\widehat{b}}\right\}\underline{\widehat{b}}^{\dagger}: &\longrightarrow \left[\underline{\underline{\widetilde{\sigma}}}^{(s)}+2\underline{\underline{\widetilde{\sigma}}}\frac{\overleftrightarrow{\partial}}{\partial\underline{\underline{\sigma}}}\underline{\underline{\sigma}}\right]P\,,\\
:\underline{\widehat{b}}\left\{\underline{\widehat{b}}^{\dagger}\widehat{\rho}\right\}: &\longrightarrow \left[\underline{\underline{\widetilde{\sigma}}}^{(s)}+2\underline{\underline{\sigma}}\frac{\overleftrightarrow{\partial}}{\partial\underline{\underline{\sigma}}}\underline{\underline{\widetilde{\sigma}}}\right]P\,,\\
\left\{\widehat{\rho}\,\underline{\widehat{b}}\,\underline{\widehat{b}}^{\dagger}\right\} &\longrightarrow \left[-\underline{\underline{\widetilde{\sigma}}}^{(s)}+2\underline{\underline{\widetilde{\sigma}}}\frac{\overleftrightarrow{\partial}}{\partial\underline{\underline{\sigma}}}\underline{\underline{\widetilde{\sigma}}}\right]P\,.
\end{aligned}
\tag{4.8}
$$

Here, $\underline{\underline{\widetilde{\sigma}}}=\underline{\underline{I}}-\underline{\underline{\sigma}}$, and $\underline{\underline{\sigma}}^{(s)}=\frac{1}{2}\left(\underline{\underline{\sigma}}-\underline{\underline{\sigma}}^{+}\right)$. The notation $\frac{\overleftrightarrow{\partial}}{\partial x}$ indicates a differentiation on both left and right sides with the ordering of matrix multiplication preserved, so that:

$$
\left[\underline{\underline{\sigma}}\frac{\overleftrightarrow{\partial}}{\partial\underline{\underline{\sigma}}}\underline{\underline{\sigma}}\right]_{\mu\nu}\equiv\frac{\partial}{\partial\sigma_{\mu\nu'}}\sigma_{\mu\nu'}\sigma_{\mu'\nu} \tag{4.9}
$$

For convenience of the reader, these identities are summarized in a more explicit form using the $M\times M$ submatrices, in the Appendix. We note here that the mixed identities involving nested orderings are not independent - one can always be obtained from the other. Also, since the kernel is analytic, the distinct analytic derivatives of the kernel are all interchangeable and lead to equivalent identities, so that generically if $\lambda_a=\lambda_a^x+i\lambda_a^y$, then $\partial/\partial\lambda_a=\partial/\partial\lambda_a^x=-i\partial/\partial\lambda_a^y$. Another freedom is that $\underline{\underline{\sigma}}$ can be replaced by $-\underline{\underline{\sigma}}^{+}$ in any of the identities.

If there are higher than quadratic terms present, the differential mappings are applied in sequence. The operator set closest to the operator $\widehat{\rho}$ leads to the innermost differential operator acting on P. Thus, for example,

$$
\begin{aligned}
:\widehat{\rho}\,\widehat{b}_{\mu}\widehat{b}_{\nu}^{\dagger}\widehat{b}_{\mu'}\widehat{b}_{\nu'}^{\dagger}: &\longrightarrow \left[\sigma_{\mu'\nu'}^{(s)}+2\frac{\partial}{\partial\sigma_{\alpha\beta}}\sigma_{\mu'\beta}\sigma_{\alpha\nu'}\right]\times\\
&\times\quad\left[\sigma_{\mu\nu}^{(s)}+2\frac{\partial}{\partial\sigma_{\gamma\delta}}\sigma_{\mu\delta}\sigma_{\gamma\nu}\right]P
\end{aligned}
\tag{4.10}
$$

For a system in which the total number is conserved, one can use the simpler thermal subset of these correspondences, i.e. including only those that contain terms that remain when all anomalous correlations vanish:

$$
\begin{aligned}
\widehat{b}_i^{\dagger}\widehat{\rho}\widehat{b}_j &\longrightarrow \left[\tilde{n}_{ij}-\frac{\partial}{\partial n_{lk}}\tilde{n}_{ik}\tilde{n}_{lj}\right]P\,,\\
\widehat{b}_i^{\dagger}\widehat{b}_j\widehat{\rho} &\longrightarrow \left[n_{ij}-\frac{\partial}{\partial n_{lk}}\tilde{n}_{ik}n_{lj}\right]P\,,\\
\widehat{\rho}\widehat{b}_i^{\dagger}\widehat{b}_j &\longrightarrow \left[n_{ij}-\frac{\partial}{\partial n_{lk}}n_{ik}\tilde{n}_{lj}\right]P\,,\\
\widehat{b}_j\widehat{\rho}\widehat{b}_i^{\dagger} &\longrightarrow \left[n_{ij}+\frac{\partial}{\partial n_{lk}}n_{ik}n_{lj}\right]P\,.
\end{aligned}
\tag{4.11}
$$

C. Fokker-Planck equation

To be able to sample the time evolution of P with stochastic phase-space equations, which is the final goal, we must have an evolution equation that is in the form of a Fokker-Planck equation, containing first and second order derivatives:

$$
\begin{aligned}
\frac{d}{dt}P(\overrightarrow{\lambda},t) \;=\; &\left[-\sum_{a=0}^{p}\frac{\partial}{\partial\lambda_a}A_a(\overrightarrow{\lambda})\right.\\
&\left.+\frac{1}{2}\sum_{a,b=0}^{p}\frac{\partial}{\partial\lambda_a}\frac{\partial}{\partial\lambda_b}D_{ab}(\overrightarrow{\lambda})\right]P(\overrightarrow{\lambda},t)\;,
\end{aligned}
\tag{4.12}
$$

where $a=0,\ldots p$ is an index that ranges over all the variables in the phase space. The matrix D_{ab} must be positive-definite when the Fokker-Planck equation is written in terms of real variables. Fortunately, the fact that the representation kernel $\widehat{\Lambda}(\overrightarrow{\lambda})$ is analytic in the phase-space variables $\overrightarrow{\lambda}$ means that the matrix D_{ab} can *always* be chosen positive-definite after it is divided into real and imaginary parts[18], through appropriate choices of the equivalent analytic forms $\partial/\partial\lambda_a=\partial/\partial\lambda_a^x=-i\partial/\partial\lambda_a^y$.

A Monte-Carlo type sampling of Eq. (4.12) can be realised by integrating the Ito stochastic equations

$$
d\lambda_a(t) \;=\; A_a(\overrightarrow{\lambda})\,dt+\sum_b B_{ab}(\overrightarrow{\lambda})\,dW_b(t)\,, \tag{4.13}
$$

where $dW_b(t)$ are Weiner increments, obeying $\langle dW_b(t)\,dW_{b'}(t')\rangle \;=\; \delta_{b,b'}\delta(t-t')dt$, i. e. Gaussian white noise. The noise matrix B_{ab} is related to the diffusion matrix by $D_{ab}=\sum_c B_{ac}B_{bc}$. This equation is directly equivalent to a path-integral in phase-space, so that the procedures outlined here can be regarded as a route to obtaining a path-integral without Grassmann variables.

Auxiliary field methods[37] can also be used to obtain a non-Grassmann path integral, but these are generally much more restrictive.

D. Stochastic gauges

The final phase-space equations are far from being unique. This freedom in the final form arises from different choices that are made at different points in the procedure. The choices at some points are constrained by the need to generate a genuine Fokker-Planck equation with a positive-definite diffusion matrix and vanishing boundary terms. Other than this, the choices are in principle free; they affect the final stochastic behaviour without changing observable moments. They are thus a stochastic analogue of a gauge choice in field theories, and a good choice of stochastic gauge can dramatically improve the performance of the simulations[32].

Because the Gaussian basis is analytic, methods previously used for the (bosonic) stochastic gauge positive-P representation are therefore applicable[32,41,42]. In the fermionic case there are three sources of gauge freedom:

1. Fermi gauges

For fermionic systems there is a freedom in the choice of operator correspondences, arising from vanishing operator products; any term involving a square of a fermion operator, like $\widehat{a}_i^2\widehat{O}$, is zero. Terms like this (and products of such terms), can be added to the Hamiltonian or Liouville equation without modifying the density matrix. The corresponding additional differential terms may not vanish, hence generating a different but equivalent stochastic equation. Such a fermionic stochastic gauge is necessary to avoid complex weights in imaginary-time simulations of interacting systems, such as the Hubbard model[29].

2. Diffusion gauges

Diffusions gauges arise from the fact that the matrix square root $D_{ab} = \sum_c B_{ac}B_{bc}$ has multiple solutions, especially if one notes that there is no restriction on the second dimension of B_{ab}. This changes the stochastic noise term and can lead to a reduction in sampling error[42].

3. Drift gauge

Drift gauges are obtained by trading off trajectory weight against trajectory direction. The possibility for drift gauges arises from the weight Ω in the density-operator expansion. The first of the correspondences in Eq. (4.8) can be used to convert drift terms for the phase-space variables into diffusion terms for the weight[19]. As a result, one can add an arbitrary gauge $g_a(\overrightarrow{\lambda})$, of the same dimension as the noise vector. Assuming $B_{0b} = 0$, and using Einstein summation conventions, this leads to:

$$\begin{aligned} d\Omega(t) &= A_0 dt + \Omega g_b dW_b(t)\,, \\ d\lambda_a(t) &= A_a\, dt + B_{ab}\,[\,dW_b(t) - g_b dt\,]\,. \end{aligned} \tag{4.14}$$

Previous work[32,41] has shown that drift gauges can remove boundary terms in bosonic positive-P representation by stabilizing deterministic trajectories.

V. EXAMPLES

The virtue of phase-space representation is that while Hilbert space dimension grows exponentially with the number of modes M, the phase-space dimension only grows quadratically. Thus, for example, a problem involving $M = 1000$ fermion modes has a Hilbert space dimension of $D = 2^{1000} = 10^{103}$ dimensions. This is larger than the number of particles in the observable universe (which is perhaps 10^{85} by current astrophysical reckoning). By contrast, the fermion phase-space dimension is 4×10^6. While large, this is not astronomical.

Hamiltonians and general time-evolution equations that are only quadratic in the Fermi ladder operators, i. e. constructed from one-body operators, will map to a Fokker-Planck equation that contains only first order derivatives. The evolving quantum state can thus be sampled by a single, deterministic trajectory. More generally, quartic terms and cubic terms (if Bose operators are included) can also be handled, and these result in stochastic equations or their equivalent path integrals.

Examples of how some typical Fermi problems are mapped into phase-space equations are given as follows.

A. Free gas

As an example of quadratic evolution, consider the thermal equilibrium calculation for a gas of noninteracting particles. The governing Hamiltonian (including the chemical potential) is always diagonalizable, and can be written as:

$$\widehat{H} = \widehat{\mathbf{b}}^\dagger \boldsymbol{\omega}\, \widehat{\mathbf{b}}\,, \tag{5.1}$$

where $\omega_{ij} = \delta_{ij}\omega_j$are the single-particle energies. The grand canonical distribution at temperature $T = 1/k_B\tau$ is found from the equation

$$\frac{\partial}{\partial\tau}\widehat{\rho} = -\frac{1}{2}\left(\widehat{\mathbf{b}}^\dagger\boldsymbol{\omega}\,\widehat{\mathbf{b}}\,\widehat{\rho} + \widehat{\rho}\,\widehat{\mathbf{b}}^\dagger\boldsymbol{\omega}\,\widehat{\mathbf{b}}\right). \tag{5.2}$$

Now this master equation can be mapped to an equivalent equation for the the distribution P by use of the thermal correspondences in Eq. (1). However, because the solution is an unnormalised density operator, there will be zeroth-order terms in the equation. We can convert such terms to first order by applying the weight (Ω)

identity in Eq. (4.8), thus obtaining the Fokker-Planck equation

$$\frac{\partial P}{\partial \tau} = \sum_k \omega_k \left[\frac{\partial}{\partial n_k}(1-n_k) + \frac{\partial}{\partial \Omega}\Omega \right] n_k P \ . \quad (5.3)$$

This Fokker-Planck equation with first-order derivatives corresponds to deterministic characteristic equations:

$$\dot{\Omega} = -\sum_k \omega_k \Omega n_k \ , \quad (5.4)$$

$$\dot{n}_k = -\omega_k n_k \left(1-n_k\right) \ . \quad (5.5)$$

Integrating the deterministic equation for the mode occupation n_k leads to the usual Fermi-Dirac distribution:

$$n_k = \frac{1}{e^{\omega_k \tau}+1} \ . \quad (5.6)$$

From integration of the weight equation, one finds that that normalisation of the density operator is

$$\mathrm{Tr}\left[\widehat{\rho}_u\right] = \Omega(\tau) = \Omega_0 \Pi_k e^{-\omega_k n_k \tau} \ , \quad (5.7)$$

i. e. the weight decays exponentially, at a rate given by the total energy.

B. General quadratic evolution

More generally, one can have a quadratic Liouville operator in situations involving non-thermal terms like $\hat{b}_i \hat{b}_j$. This can occur for, example, when fermion pairs are generated from molecule or exciton dissociation. These are even associated with certain spin-chain problems[43], where the Jordan-Wigner theorem is used to transform spins to fermion operators. Other quadratic Liouville operators are commonly found in cases involving coupling to reservoirs[40].

The generic phase-space equations for a general Fermi system with a quadratic Liouville operator can be easily obtained, for evolution both through time and through inverse temperature. The most general master equation that covers both kinds of evolution can be written

$$\frac{d}{d\tau}\widehat{\rho} = K\widehat{\rho} - \frac{1}{2}\sum_{\mu\nu}\Big(\mathcal{A}_{\nu\mu} : \widehat{b}_\mu \widehat{b}^\dagger_\nu \widehat{\rho} : + \mathcal{B}_{\nu\mu}\left\{ \widehat{b}_\mu \widehat{b}^\dagger_\nu \widehat{\rho} \right\} + \mathcal{C}_{\nu\mu} : \left\{ \widehat{\rho} \widehat{b}_\mu \right\} \widehat{b}^\dagger_\nu : + \mathcal{C}^*_{\mu\nu}\left\{ : \widehat{\rho} \widehat{b}_\mu : \widehat{b}^\dagger_\nu \right\} \Big) , \quad (5.8)$$

where the elements of $2M \times 2M$ matrices $\underline{\underline{\mathcal{A}}}$, $\underline{\underline{\mathcal{B}}}$ and $\underline{\underline{\mathcal{C}}}$ are determined by the coefficients of the Hamiltonian or master equation. By applying the mappings of Eq. (4.8), we find the evolution of the covariance matrix to be:

$$\frac{d}{d\tau}\underline{\underline{\sigma}} = \underline{\underline{\sigma}}\,\underline{\underline{\mathcal{A}}}\,\underline{\underline{\sigma}} + \underline{\underline{\widetilde{\sigma}}}\,\underline{\underline{\mathcal{B}}}\,\underline{\underline{\widetilde{\sigma}}} + \underline{\underline{\sigma}}\,\underline{\underline{\mathcal{C}}}\,\underline{\underline{\widetilde{\sigma}}} + \underline{\underline{\widetilde{\sigma}}}\,\underline{\underline{\mathcal{C}}}^\dagger\,\underline{\underline{\sigma}}, \quad (5.9)$$

This equation simply corresponds to the characteristic or drift equations given by the vector $\vec{A}$ in the Ito stochastic equation (4.13), and in these cases there is no diffusion or stochastic term. Unlike a conventional path integral, we see that a quadratic Hamiltonian or Liouville equation simply results in a noise-free, deterministic trajectory on phase space. For deterministic evolution such as this, the weight Ω does not affect physical observables, so we do not consider it here.

In the examples that follow, we assume for simplicity (but without loss of generality) that the constant matrices have been chosen with hermitian anti-symmetry such that:

$$\begin{aligned} \underline{\underline{A}} &= -\underline{\underline{A}}^+ \\ \underline{\underline{B}} &= -\underline{\underline{B}}^+ \\ \underline{\underline{C}}^\dagger &= -\underline{\underline{C}}^+ \ . \end{aligned} \quad (5.10)$$

1. Temperature evolution

For temperature evolution, the structure of the master equation (Eq. (4.4)) is such that $\underline{\underline{A}} = \underline{\underline{B}}$ and $\underline{\underline{\mathcal{C}}} = \underline{\underline{\mathcal{C}}}^\dagger$, giving the simpler result:

$$\frac{d}{d\tau}\underline{\underline{\sigma}} = \frac{1}{2}\left(\underline{\underline{I}} - 2\underline{\underline{\sigma}}\right)\underline{\underline{T}}\left(\underline{\underline{I}} - 2\underline{\underline{\sigma}}\right) + \underline{\underline{\sigma}}^0, \quad (5.11)$$

where we have introduced:

$$\begin{aligned} \underline{\underline{T}} &= \underline{\underline{\mathcal{B}}} - \underline{\underline{\mathcal{C}}} \\ \underline{\underline{\sigma}}^0 &= \frac{1}{4}\underline{\underline{I}}\left(\underline{\underline{\mathcal{B}}} - 2\underline{\underline{\mathcal{C}}}\right)\underline{\underline{I}} \ . \end{aligned} \quad (5.12)$$

For the case of a number conserving Hamiltonian $H = \mathbf{b}^\dagger \boldsymbol{\omega} \mathbf{b}$, we find that $\underline{\underline{B}} = 0$ and

$$\underline{\underline{\mathcal{C}}} = \frac{1}{2}\begin{bmatrix} -\boldsymbol{\omega}^T & \mathbf{0} \\ \mathbf{0} & \boldsymbol{\omega} \end{bmatrix} . \quad (5.13)$$

The phase-space equations then reduce to

$$\frac{d}{d\tau}\mathbf{n} = -\frac{1}{2}\left(\mathbf{n}\boldsymbol{\omega}\widetilde{\mathbf{n}} + \widetilde{\mathbf{n}}\boldsymbol{\omega}\mathbf{n}\right), \quad (5.14)$$

which reproduces the free gas example above.

2. Dynamical evolution

For time evolution, with possible coupling to the environment, there is a different symmetry to the master equation (Eq. (4.3)) that means that $\underline{\underline{\mathcal{A}}} + \underline{\underline{\mathcal{B}}} - \underline{\underline{\mathcal{C}}} - \underline{\underline{\mathcal{C}}}^\dagger = \underline{\underline{0}}$. A formal solution to the phase-space equations can now be explicitly written down:

$$\underline{\underline{\sigma}}(t) = \exp\left(-\underline{\underline{U}}^\dagger t\right)\left(\underline{\underline{\sigma}}(0) - \underline{\underline{\sigma}}^\infty\right)\exp\left(-\underline{\underline{U}} t\right) + \underline{\underline{\sigma}}^\infty, \quad (5.15)$$

where $\underline{\underline{U}} = \left(\underline{\underline{\mathcal{B}}} - \underline{\underline{\mathcal{C}}}\right) \underline{\underline{I}}$ and where $\underline{\underline{\sigma}}^{\infty}$ satisfies:

$$\underline{\underline{I}}\,\underline{\underline{\mathcal{B}}}\,\underline{\underline{I}} = \underline{\underline{U}}^{\dagger}\,\underline{\underline{\sigma}}^{\infty} + \underline{\underline{\sigma}}^{\infty}\underline{\underline{U}}\,. \tag{5.16}$$

To illustrate the physical meaning of these matrices, we consider the simplest model of a small quantum dot coupled to a zero-temperature reservoir:

$$\dot{\widehat{\rho}} \;=\; -i\omega\widehat{b}^{\dagger}\widehat{b}\widehat{\rho} + i\omega\widehat{\rho}\widehat{b}^{\dagger}\widehat{b} + \gamma\left(\widehat{b}\widehat{\rho}\widehat{b}^{\dagger} - \frac{1}{2}\widehat{b}^{\dagger}\widehat{b}\widehat{\rho} - \frac{1}{2}\widehat{\rho}\widehat{b}^{\dagger}\widehat{b}\right). \tag{5.17}$$

In terms of the general form, this corresponds to $\underline{\underline{\mathcal{A}}} = \underline{\underline{0}}$, $\underline{\underline{\mathcal{B}}} = \gamma\underline{\underline{I}}$, and

$$\underline{\underline{\mathcal{C}}} \;=\; \left[\begin{array}{cc} -i\omega - \frac{1}{2}\gamma & 0 \\ 0 & -i\omega + \frac{1}{2}\gamma \end{array}\right]. \tag{5.18}$$

The general solution then reduces to

$$\begin{aligned}\underline{\underline{\sigma}}(t) \;&=\; \left[\begin{array}{cc} e^{-i\omega-\gamma/2} & 0 \\ 0 & e^{i\omega+\gamma/2} \end{array}\right]\left(\underline{\underline{\sigma}}(0) - \underline{\underline{I}}\right) \\ &\quad\times\left[\begin{array}{cc} e^{i\omega-\gamma/2} & 0 \\ 0 & e^{-i\omega-\gamma/2} \end{array}\right] + \underline{\underline{I}},\end{aligned} \tag{5.19}$$

which implies that the density decays as $n(t) = e^{-\gamma t}n(0)$, as expected.

The solution to a multimode quantum dot model also follows from Eq. (5.15). The relevant master equation is

$$\begin{aligned}\dot{\widehat{\rho}} \;&=\; -i\omega_{ji}\widehat{b}_i^{\dagger}\widehat{b}_j\widehat{\rho} + i\omega_{ji}\widehat{\rho}\widehat{b}_i^{\dagger}\widehat{b}_j \\ &\quad+\gamma_{ij}\left(\widehat{b}_i\widehat{\rho}\widehat{b}_j^{\dagger} - \frac{1}{2}\widehat{b}_j^{\dagger}\widehat{b}_i\widehat{\rho} - \frac{1}{2}\widehat{\rho}\widehat{b}_j^{\dagger}\widehat{b}_i\right),\end{aligned} \tag{5.20}$$

for which the evolution matrix is

$$\underline{\underline{U}} \;=\; \left[\begin{array}{cc} e^{-i\boldsymbol{\omega}^T+\boldsymbol{\gamma}^T/2} & \mathbf{0} \\ \mathbf{0} & e^{i\boldsymbol{\omega}+\boldsymbol{\gamma}/2} \end{array}\right]. \tag{5.21}$$

Physically, this corresponds, as expected, to damped oscillatory behavior (taking $\boldsymbol{\gamma}$ to be positive definite) in the moments:

$$\begin{aligned}\mathbf{n} \;&=\; e^{i\boldsymbol{\omega}-\boldsymbol{\gamma}/2}\mathbf{n}(0)e^{-i\boldsymbol{\omega}-\boldsymbol{\gamma}/2}, \\ \mathbf{m} \;&=\; e^{-i\boldsymbol{\omega}^T-\boldsymbol{\gamma}^T/2}\mathbf{m}(0)e^{-i\boldsymbol{\omega}-\boldsymbol{\gamma}/2}.\end{aligned} \tag{5.22}$$

Here, of course, there are no electron-electron interactions included. However, such interactions can be dealt with via a stochastic sampling methods, as we show in the next section.

C. Interacting gas

1. Two-body interactions

For systems of particles with two-body interactions, the Gaussian representation gives nonlinear, stochastic phase-space equations, which must be solved numerically. Consider a two-body interaction of the form:

$$\widehat{H}_2 \;=\; \sum_{ij} U_{ij}\widehat{n}_i\widehat{n}_j\,,$$

where $\widehat{n}_{ij} = \widehat{a}_i^{\dagger}\widehat{a}_j$. For a number-conserving system, we can use correspondences of Eq. (4.11) to generate a Fokker-Planck equation for the grand canonical evolution. The diffusion matrix $D_{u,v}$ in this equation is

$$\begin{aligned}D_{ij,kl} \;&=\; -\sum_{pq} U_{pq}\left\{n_{ip}\widetilde{n}_{pj}n_{kq}\widetilde{n}_{ql}\right. \\ &\quad\left.+\widetilde{n}_{ip}n_{pj}\widetilde{n}_{kq}n_{ql}\right\}.\end{aligned} \tag{5.23}$$

Suppose that the interaction matrix U_{pq} is negative-definite, such that we can write it as a sum of negative squares: $U_{pq} = -\sum_{\alpha} b_{p,\alpha}b_{q,\alpha}$. Then the diffusion matrix is positive definite, as it can be written in the form:

$$D_{ij,kl} \;=\; \sum_{\alpha}\left\{B^{(1)}_{ij,\alpha}B^{(1)}_{kl,\alpha} + B^{(2)}_{ij,\alpha}B^{(2)}_{kl,\alpha}\right\}, \tag{5.24}$$

where the noise matrices are:

$$\begin{aligned}B^{(1)}_{ij,\alpha} \;&=\; \sum_{p} b_{p,\alpha}n_{ip}\widetilde{n}_{pj}\,, \\ B^{(2)}_{ij,\alpha} \;&=\; \sum_{p} b_{p,\alpha}\widetilde{n}_{ip}n_{pj}\,.\end{aligned} \tag{5.25}$$

Thus for an interaction of this type, the noise terms in the final stochastic equations will be real. The form of noise terms for a more general interaction is considered in[46].

2. Hubbard model

As an example, we apply the representation to the Hubbard model, which is the simplest nontrivial model for strongly interacting fermions on a lattice. It is an important system in condensed matter physics, with relevance to the theory of high-temperature superconductors[26], and in ultracold atomic physics. The full phase-diagram in two dimensions is not fully understood as yet. Due to developments in atomic lattices, this model is directly experimentally accessible[6,44].

The Hamiltonian for the model is[30]:

$$H(\widehat{\mathbf{n}}_1, \widehat{\mathbf{n}}_{-1}) \;=\; -\sum_{ij,\sigma} t_{ij}\widehat{n}_{ij,\sigma} + U\sum_{j}\widehat{n}_{jj,1}\widehat{n}_{jj,-1}, \tag{5.26}$$

where $\widehat{n}_{ij,\sigma} = \widehat{a}^{\dagger}_{i,\sigma}\widehat{a}_{j,\sigma} = \{\widehat{\mathbf{n}}_{\sigma}\}_{ij}$. The index σ denotes spin (± 1), the indices i, j label lattice location. Here $t_{ij} = t$ if the i, j correspond to nearest neighbour sites, $t_{ij} = \mu$ if $i = j$ and is otherwise 0. The chemical potential μ is included to control the total particle number.

Because the Hubbard model conserves total number and spin, one can map this problem to a reduced phase space of $\lambda = (\Omega, n_{ij,1}, n_{ij,-1})$. Thus the simpler mappings of Eq. (4.11) can be used for each spin component. The one-body terms generate drift terms only, and can be dealt with as above. The two-body terms generate both drift and diffusion terms. Applying the mappings directly to the Hubbard model as written above, we obtain the diffusion matrix

$$\begin{aligned} D_{ij\sigma,kl\sigma'} &= -U\delta_{\sigma,-\sigma'}\sum_p \{n_{ip\sigma}\widetilde{n}_{pj\sigma}n_{kp\sigma'}\widetilde{n}_{pl\sigma'} \\ &\quad +\widetilde{n}_{ip\sigma}n_{pj\sigma}\widetilde{n}_{kp\sigma'}n_{pl\sigma'}\}, \end{aligned} \tag{5.27}$$

which, because it has zeros on the diagonal, cannot be put into a positive definite form with real variables.

However, using the anticommuting properties of the Fermi operators, we can rewrite the interaction term in the Hubbard Hamiltonian as

$$\begin{aligned} H_I &= -\frac{|U|}{2}\sum_j :\left(\widehat{n}_{jj,1} - S\widehat{n}_{jj,-1}\right)^2: \\ &= \sum_j U_{i\sigma,j\sigma'} :\widehat{n}_{ii,\sigma}\widehat{n}_{jj,\sigma'} \end{aligned} \tag{5.28}$$

where $S = U/|U| = \pm 1$. Now in this form, the interaction matrix is negative definite:

$$\begin{aligned} U_{i\sigma,j\sigma'} &= -\frac{|U|}{2}\delta_{ij}\left(\delta_{\sigma,\sigma'} - S\delta_{\sigma,-\sigma'}\right) \\ &= -\frac{|U|}{2}\sum_k \delta_{i,k}\sigma^s\delta_{j,k}\sigma'^s, \end{aligned} \tag{5.29}$$

where $s = (S+1)/2$, so that $s = 0$ for the attractive case and $s = 1$ for the repulsive case.

From Eq. (5.24) the diffusion matrix is positive definite, with corresponding noise matrices:

$$\begin{aligned} B^{(1)}_{ij\sigma,\alpha} &= \sqrt{|U|/2}\sigma^s n_{i\alpha}\widetilde{n}_{\alpha j}, \\ B^{(2)}_{ij\sigma,\alpha} &= \sqrt{|U|/2}\sigma^s \widetilde{n}_{i\alpha}n_{\alpha j}. \end{aligned} \tag{5.30}$$

With this choice of noise terms, the final phase-space equations are, in Itô form,

$$\frac{d\mathbf{n}_\sigma}{d\tau} = \frac{1}{2}\left\{\tilde{\mathbf{n}}_\sigma \boldsymbol{T}^{(1)}_\sigma \mathbf{n}_\sigma + \mathbf{n}_\sigma \boldsymbol{T}^{(2)}_\sigma \tilde{\mathbf{n}}_\sigma\right\}, \tag{5.31}$$

where we have introduced the stochastic propagation matrix:

$$T^{(r)}_{ij,\sigma} = t_{ij} - \delta_{ij}\left\{Un_{jj,-\sigma} + \sigma^s\xi^{(r)}_j\right\}. \tag{5.32}$$

The real Gaussian noise $\xi^{(r)}_j(\tau)$ is defined by the correlations

$$\left\langle \xi^{(r)}_j(\tau)\,\xi^{(r')}_{j'}(\tau')\right\rangle = 2|U|\,\delta(\tau-\tau')\delta_{jj'}\delta_{rr'}.$$

Because the diffusion can be realised in terms of real noise, the phase-space equations will not be driven off the real manifold. This has an important implication for the weight Ω, which enters the problem because the solution will be an unnormalised density operator. The weights for each trajectory evolve as physically expected for energy-weighted averages, with weights depending exponentially on the inverse temperature τ and the effective trajectory Hamiltonian H:

$$\frac{d\Omega}{d\tau} = -\Omega H(\mathbf{n}_1, \mathbf{n}_{-1}).$$

Because the equations for the phase-space variables $n_{ij,\sigma}$ are all real, the weights will all remain positive, thereby eliminating the traditional manifestation of the sign problem.

This method can calculate any correlation function, at any temperature, to the precision allowed by the sampling error and subject to there being no boundary terms in Eq. (4.6). Preliminary simulations in one[45], two[29] and three dimensions showed that sampling error is well-controlled, even for very low temperatures. However, more extensive simulations of the 2D Hubbard model have shown that, at half filling, certain correlation functions do not appear to converge to the correct zero-temperature results at these very low temperatures[46]. Because the Gaussian basis does not possess many of the symmetries of the Hubbard model, they must be restored in the distribution over Gaussian basis elements. For finite sampling, this restoration may be incomplete, giving the departure from exact results at low temperatures. It has been shown that the correct results can be obtained by applying a projection onto a symmetric subspace[46]. There may also be systematic errors if boundary terms are present. Both of these possibilities imply that further optimization via stochastic gauge choices may be required to keep the low-temperature distributions compact, free from tails and from features that would lead to biasing.

3. Drift gauges

For the Hubbard model, we can modify the drift part according to Eq. (4.14) by adding a term $\mathbf{G}_\sigma$ to the stochastic propagation matrices $\mathbf{T}^{(r)}_\sigma$. Because of the diagonal nature of the noise terms, the added term will also be diagonal: $G_{ij,\sigma} = \delta_{ij}G_{j,\sigma}$. The additional diffusion term in the weight equation is then

$$\left(\frac{d\Omega}{d\tau}\right)_g = \frac{\Omega}{2|U|}\sum_{jr\sigma}\sigma^s G_{j,\sigma}\xi^{(r)}_j. \tag{5.33}$$

The choice of gauge term $\mathbf{G}_\sigma$ is guided on the one hand by the need to ensure the phase-space distribution remains bounded and on the other by the requirement of introducing only the minimum amount of diffusion into the weight. The function should thus act only when necessary to control large trajectories and should be zero otherwise.

The diagonal form of gauge term possible is able to remove instabilities in the Hubbard equations that are directly due to the interaction term U. However, instabilities may still arise from the coupling terms t_{ij}, even though they are of lower order. Thus it may be necessary to introduce weaker, off-diagonal gauge terms. This in turn requires additional, off-diagonal noise terms in the propagation matrix. Such noises can be introduced by use of additional Fermi gauges. For example, the vanishing term[47]

$$0 \;=\; \sum_{ij\sigma} \frac{1}{2} V_{ji,\sigma} \left\{ (\delta_{ij} - \widehat{n}_{ij,\sigma})\, \widehat{n}_{ij,\sigma} \widehat{\rho} + \widehat{\rho}\, \widehat{n}_{ij,\sigma}\, (\delta_{ij} - \widehat{n}_{ij,\sigma}) \right\}, \tag{5.34}$$

where $V_{ij,\sigma}$ are positive numbers, gives the additional stochastic contribution to the propagation matrix:

$$T^{(r)}_{ij,\sigma} \;\rightarrow\; T^{(r)}_{ij,\sigma} + \zeta^{(r)}_{ij,\sigma}(\tau)\,, \tag{5.35}$$

where the new noises $\zeta^{(r)}_{ij,\sigma}(\tau)$ have the correlations

$$\left\langle \zeta^{(r)}_{ij}(\tau)\, \zeta^{(r')}_{i'j'}(\tau') \right\rangle \;=\; 4V_{ij,\sigma} \delta(\tau - \tau') \delta_{ii'} \delta_{jj'} \delta_{rr} \tag{5.36}$$

We can now introduce arbitrary off-diagonal gauge terms $G_{ij,\sigma}$ into the propagation matrix, with the corresponding diffusion term in the weight equation

$$\left(\frac{d\Omega}{d\tau} \right)_g \;=\; -\Omega \sum_{ijr\sigma} G_{ij,\sigma} \zeta^{(r)}_{ij} / 4V_{ij,\sigma}\,. \tag{5.37}$$

Again there is a trade-off between gauge strength and additional diffusion. But there is also a freedom (in the choice of $V_{ij,\sigma}$) as to whether the noise appears in the weight equation or in the propagation matrix.

With such a combination of Fermi and drift gauges, it is possible to introduce terms to stabilise the drift evolution of any of the phase-space variables $n_{ij,\sigma}$, and so maintain a bounded phase-space distribution.

VI. CONCLUSION

In summary, we have introduced a phase-space representation for many-body fermionic states, enabling new types of first-principles calculations and simulations of highly correlated systems. Many-body systems with one- and two-body interactions can be solved by use of stochastic sampling methods, since they can be transformed into a second-order Fokker-Planck equation, provided a suitable stochastic gauge is chosen to ensure that the distribution remains sufficiently bounded.

These techniques are potentially applicable to a wide range of fermionic problems, including both real-time and finite temperature calculations. Generalized master equations for non-equilibrium fermionic open systems coupled to reservoirs are a particularly suitable type of application. We have given examples of the use of fermionic differential identities to transform multi-mode master equations into deterministic phase-space equations, although more general interactions typically lead to stochastic equations. These equations have exponentially less complexity than the full Hilbert space equations, are generally simpler to solve than path integrals, and never involve either Grassmann variables or determinants.

The application to the Hubbard model demonstrates the immediate utility of the Gaussian method to solving long-standing problems in many-body quantum physics, provided suitable gauges can be found to ensure that boundary terms to not arise. Rapid experimental advances in the area of ultra-cold fermionic atoms[5] mean that direct and quantitative tests of precise theoretical predictions should be feasible in the near future. Demonstration of a quantum degenerate Fermi gas in a lattice has already taken place[6].

The general technique established here potentially also has broad applicability in many other areas of quantum many-body theory and quantum field theory.

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APPENDIX

It is sometimes more convenient to work with explicit $\mathbf{n}, \mathbf{m}, \mathbf{m}^+$submatrices rather than the total covariance. In fully indexed notation, using the $M \times M$ submatrices, the Fermi operator correspondences (Eq. (4.8))become:

$$
\begin{aligned}
\widehat{b}_i^\dagger \widehat{b}_j \widehat{\rho} &\longrightarrow \left[n_{ij} - \frac{\partial}{\partial n_{lk}} \left\{ n_{lj}\tilde{n}_{ik} + m^+_{li} m_{jk} \right\} - \frac{\partial}{\partial m_{lk}} \left\{ m_{lj}\tilde{n}_{ik} + \tilde{n}_{il} m_{jk} \right\} + \frac{\partial}{\partial m^+_{lk}} \left\{ n_{lj} m^+_{ik} + m^+_{li} n_{kj} \right\} \right] P \,, \\
\widehat{\rho} \widehat{b}_i^\dagger \widehat{b}_j &\longrightarrow \left[n_{ij} - \frac{\partial}{\partial n_{lk}} \left\{ \tilde{n}_{lj} n_{ik} + m^+_{li} m_{jk} \right\} + \frac{\partial}{\partial m_{lk}} \left\{ m_{lj} n_{ik} + n_{il} m_{jk} \right\} - \frac{\partial}{\partial m^+_{lk}} \left\{ \tilde{n}_{lj} m^+_{ik} + m^+_{li} \tilde{n}_{kj} \right\} \right] P \,, \\
\widehat{b}_i^\dagger \widehat{\rho} \widehat{b}_j &\longrightarrow \left[\tilde{n}_{ij} - \frac{\partial}{\partial n_{lk}} \left\{ \tilde{n}_{lj}\tilde{n}_{ik} - m^+_{li} m_{jk} \right\} + \frac{\partial}{\partial m_{lk}} \left\{ m_{lj}\tilde{n}_{ik} + \tilde{n}_{il} m_{jk} \right\} + \frac{\partial}{\partial m^+_{lk}} \left\{ \tilde{n}_{lj} m^+_{ik} + m^+_{li} \tilde{n}_{kj} \right\} \right] P \,, \\
\widehat{b}_j \widehat{\rho} \widehat{b}_i^\dagger &\longrightarrow \left[n_{ij} - \frac{\partial}{\partial n_{lk}} \left\{ m^+_{li} m_{jk} - n_{lj} n_{ik} \right\} + \frac{\partial}{\partial m_{lk}} \left\{ m_{lj} n_{ik} + n_{il} m_{jk} \right\} + \frac{\partial}{\partial m^+_{lk}} \left\{ n_{lj} m^+_{ik} + m^+_{li} n_{kj} \right\} \right] P \,, \\
\widehat{b}_i \widehat{b}_j \widehat{\rho} &\longrightarrow \left[m_{ij} - \frac{\partial}{\partial n_{lk}} \left\{ n_{li} m_{jk} - n_{lj} m_{ik} \right\} - \frac{\partial}{\partial m_{lk}} \left\{ m_{li} m_{jk} - m_{lj} m_{ik} \right\} - \frac{\partial}{\partial m^+_{lk}} \left\{ n_{lj} n_{ki} - n_{li} n_{kj} \right\} \right] P \,, \\
\widehat{\rho} \widehat{b}_i \widehat{b}_j &\longrightarrow \left[m_{ij} - \frac{\partial}{\partial n_{lk}} \left\{ \tilde{n}_{lj} m_{ik} - \tilde{n}_{li} m_{jk} \right\} - \frac{\partial}{\partial m_{lk}} \left\{ m_{li} m_{jk} - m_{lj} m_{ik} \right\} - \frac{\partial}{\partial m^+_{lk}} \left\{ \tilde{n}_{lj} \tilde{n}_{ki} - \tilde{n}_{li} \tilde{n}_{kj} \right\} \right] P \,, \\
\widehat{b}_j \widehat{\rho} \widehat{b}_i &\longrightarrow \left[m_{ij} + \frac{\partial}{\partial n_{lk}} \left\{ \tilde{n}_{li} m_{jk} + n_{lj} m_{ik} \right\} - \frac{\partial}{\partial m_{lk}} \left\{ m_{li} m_{jk} - m_{lj} m_{ik} \right\} - \frac{\partial}{\partial m^+_{lk}} \left\{ \tilde{n}_{li} n_{kj} - \tilde{n}_{lj} n_{ki} \right\} \right] P \,, \\
\widehat{b}_i^\dagger \widehat{b}_j^\dagger \widehat{\rho} &\longrightarrow \left[m^+_{ij} - \frac{\partial}{\partial n_{lk}} \left\{ m^+_{lj} \tilde{n}_{ik} - m^+_{li} \tilde{n}_{jk} \right\} - \frac{\partial}{\partial m_{lk}} \left\{ \tilde{n}_{jl} \tilde{n}_{ik} - \tilde{n}_{il} \tilde{n}_{jk} \right\} - \frac{\partial}{\partial m^+_{lk}} \left\{ m^+_{li} m^+_{jk} - m^+_{lj} m^+_{ik} \right\} \right] P \,, \\
\widehat{\rho} \widehat{b}_i^\dagger \widehat{b}_j^\dagger &\longrightarrow \left[m^+_{ij} - \frac{\partial}{\partial n_{lk}} \left\{ m^+_{li} n_{jk} - m^+_{lj} n_{ik} \right\} - \frac{\partial}{\partial m_{lk}} \left\{ n_{jl} n_{ik} - n_{il} n_{jk} \right\} - \frac{\partial}{\partial m^+_{lk}} \left\{ m^+_{li} m^+_{jk} - m^+_{lj} m^+_{ik} \right\} \right] P \,, \\
\widehat{b}_j^\dagger \widehat{\rho} \widehat{b}_i^\dagger &\longrightarrow \left[m^+_{ij} + \frac{\partial}{\partial n_{lk}} \left\{ m^+_{lj} n_{ik} + m^+_{li} \tilde{n}_{jk} \right\} - \frac{\partial}{\partial m_{lk}} \left\{ n_{il} \tilde{n}_{jk} - \tilde{n}_{jl} n_{ik} \right\} - \frac{\partial}{\partial m^+_{lk}} \left\{ m^+_{li} m^+_{jk} - m^+_{lj} m^+_{ik} \right\} \right] P \,, \qquad (1)
\end{aligned}
$$

where we have used the Einstein summation convention for repeated indices. Furthermore, we have explicitly written out the extra derivative terms that arise from the antisymmetry of $\mathbf{m}$ and $\mathbf{m}^+$, such that the summation of these terms is only for $k > l$. The factor of two difference between these equations and the full covariance equations is due to the fact that these equations correspond to a covariance which is constrained to satisfy the Hermitian anti-symmetry condition.

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